Opportunities and Challenges for Simulation at the ATF

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2019 ATF Science Planning Workshop

Collaborative efforts in accelerator modeling

Collaborations –

MHD: N. Cook & J. Carlsson (RadiaSoft), P. Tzeferacos (Chicago)

Plasma: D. Bruhwiler, N. Cook, & S. Webb (RadiaSoft), R. Lehe, & J.-L. Vay (LBNL)

Dielectrics: D. Bruhwiler & N. Cook (RadiaSoft), G. Andonian (RadiaBeam), F. Oshea (Trieste)

ML: J. Edelen, N. Cook, C. Hall, S. Webb (RadiaSoft)
K. Brown, P. Dyer (BNL), A. Edelen (SLAC)

Sirepo team: R. Nagler, P. Moeller, M. Keilman & E. Carlin (RadiaSoft)

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DE-SC0019682 (NP).

Outline

- Magnetohydrodynamics of plasma targets and lenses
  - *Channel formation for laser guiding*
  - *Active plasma lenses*
  - *Target shaping for laser plasma interactions*

- Laser- and Beam-driven accelerator simulations
  - *Hybrid dielectric wakefield acceleration schemes*
  - *Modeling of advanced ionization schemes*
  - *Beam Plasma Interactions*

- Controls Systems and Machine Learning
  - *Virtual diagnostics for electron phase space tomography*
  - *Beamline modeling and optimization*
  - *Controls interface leveraging EPICS*

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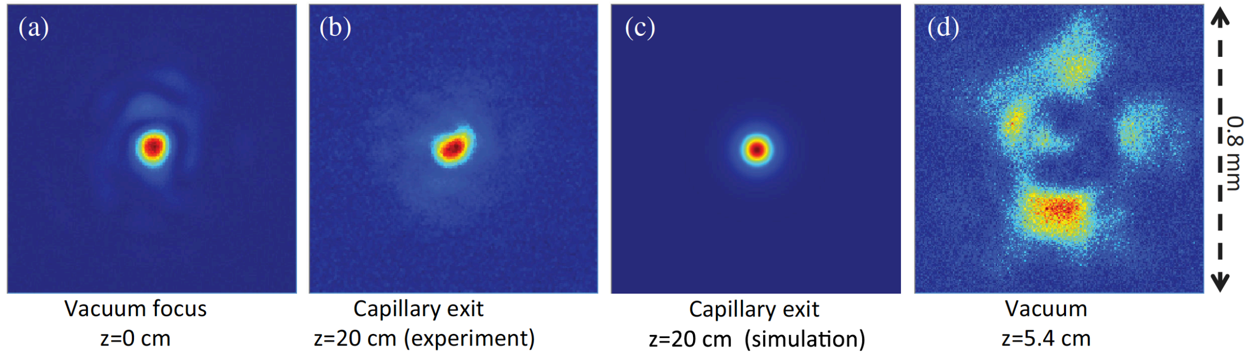
Discharge capillary plasmas enable advanced concepts

Guiding of intense pulses:

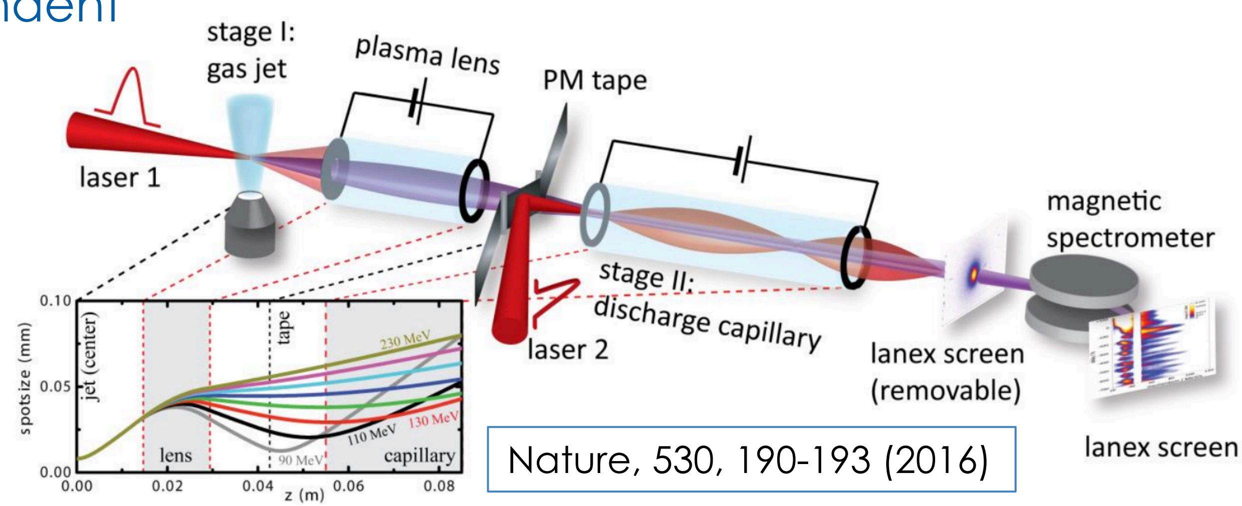
- Generate parabolic plasma channel along capillary
- Maintain laser spot over long distances



Phys. Rev. Lett. **122**, 084801 (2019)

Beam transport, focusing, and staging:

- Produce time-dependent azimuthal magnetic field across capillary cross-section
- kT/m gradients achievable



Nature, 530, 190-193 (2016)

Deconstructing a Capillary Discharge Plasma

- Narrow insulating tube with controlled gas flow
  - *Hydrogen, Helium, Argon*
  - *Length from ~1-30 cm*
    Radius from ~0.1-1 mm
- Applied voltage drives discharge
  - *Vary density, voltage to adjust*

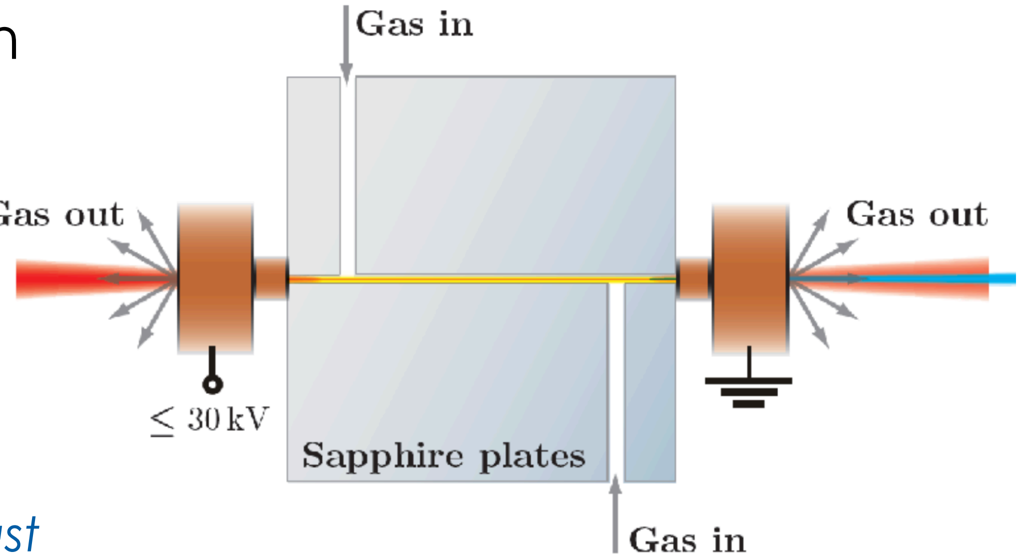
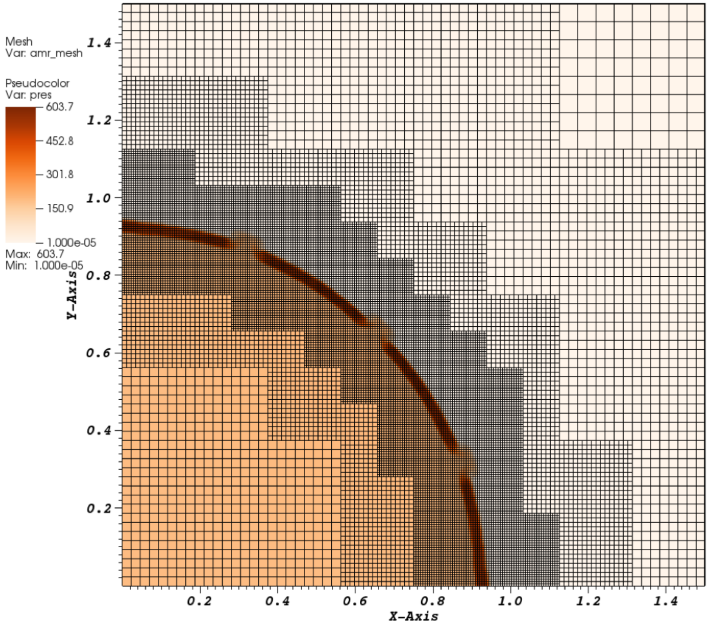


Figure Credit: Jens Osterhoff

- Many computational Complexities
  - *High Aspect Ratio*
  - *High temporal resolution required*
    - Transport timescales (0.01-10 ps) are small compared to discharge (>100 ns)
    - Magnetic field effects require explicit integration
  - *Time Dependent boundaries require special treatment*
    - Discharge representation influences choice of boundary conditions
    - Electrical and Thermal conductivities must change self-consistently

Magnetohydrodynamics modeling with FLASH



- Uniform, block-structured grid
  - *AMR with user-specified refinement*
  - *Cartesian, Spherical, Cylindrical, Polar*
- Solves 3T fluid evolution with convection

$$\left\{\begin{array}{c} \frac{\partial}{\partial t}(\rho e_\mathrm{i}) + \nabla\cdot(\rho e_\mathrm{i}\boldsymbol{v}) + P_\mathrm{i}\nabla\cdot\boldsymbol{v} = \rho\frac{c_{v,\mathrm{e}}}{\tau_{ei}}(T_\mathrm{e}-T_\mathrm{i}) \\ \frac{\partial}{\partial t}(\rho e_\mathrm{e}) + \nabla\cdot(\rho e_\mathrm{e}\boldsymbol{v}) + P_\mathrm{e}\nabla\cdot\boldsymbol{v} = \rho\frac{c_{v,\mathrm{e}}}{\tau_{ei}}(T_\mathrm{i}-T_\mathrm{e}) - \nabla\cdot\boldsymbol{q}_\mathrm{e} + Q_\mathrm{abs} - Q_\mathrm{emis} + Q_\mathrm{las} \\ \frac{\partial}{\partial t}(\rho e_\mathrm{r}) + \nabla\cdot(\rho e_\mathrm{r}\boldsymbol{v}) + P_\mathrm{r}\nabla\cdot\boldsymbol{v} = \nabla\cdot\boldsymbol{q}_\mathrm{r} - Q_\mathrm{abs} + Q_\mathrm{emis} \end{array}\right\}$$

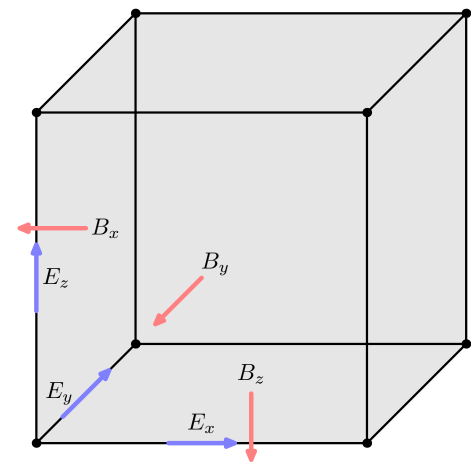
- Dissipation via conduction and heat exchange

$$\frac{\partial e_\mathrm{e}}{\partial t} = \nabla\cdot K_\mathrm{e}\nabla T_\mathrm{e} \qquad \begin{array}{l} \frac{\partial e_\mathrm{i}}{\partial t} = \frac{c_{v,\mathrm{e}}}{\tau_{ei}}(T_\mathrm{e}-T_\mathrm{i}) \\ \frac{\partial e_\mathrm{e}}{\partial t} = \frac{c_{v,\mathrm{e}}}{\tau_{ei}}(T_\mathrm{i}-T_\mathrm{e}) \end{array}$$

- Spitzer model describes plasma resistivity (and thermal conduction)

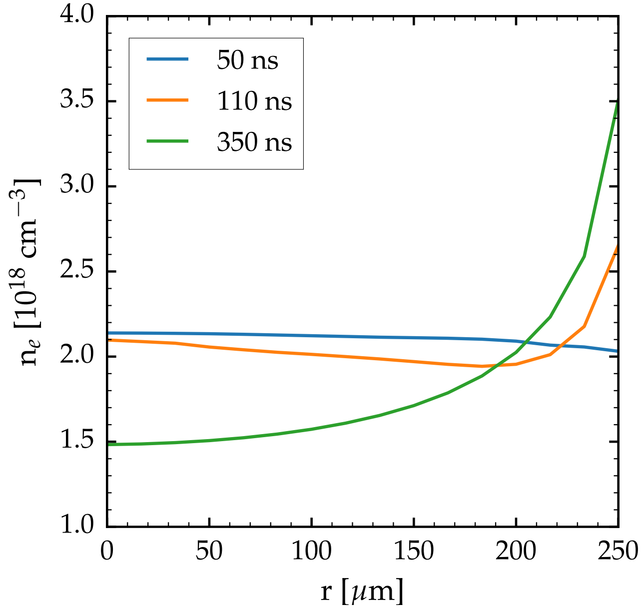
$$\eta_\perp = \frac{4\sqrt{2\pi}}{3}\frac{Ze^2 m_e^{1/2}\ln\Lambda}{(4\pi\epsilon_0)^2(k_B T_e)^{3/2}}F(Z)$$

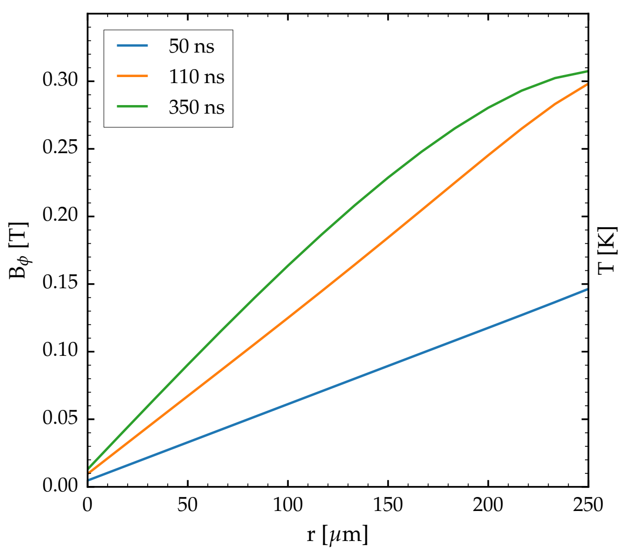
- Electromagnetic fields defined on a Yee mesh
  - *Secondary, uniform mesh overlapping fluid domain*
  - *Divergence-free condition enforced*
  - *Explicit integration scheme*

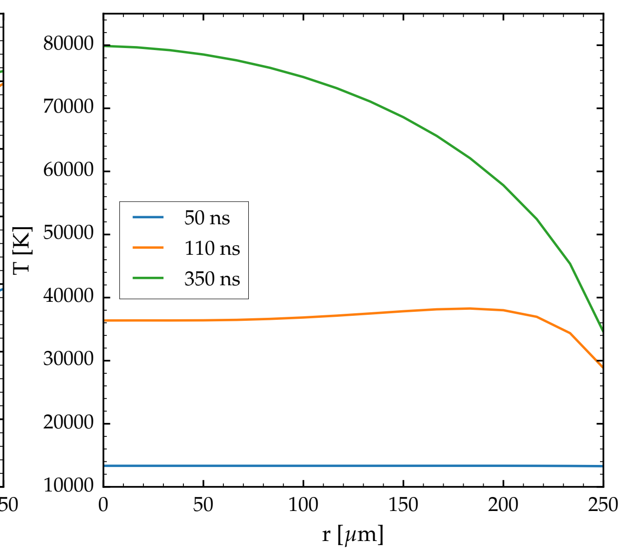


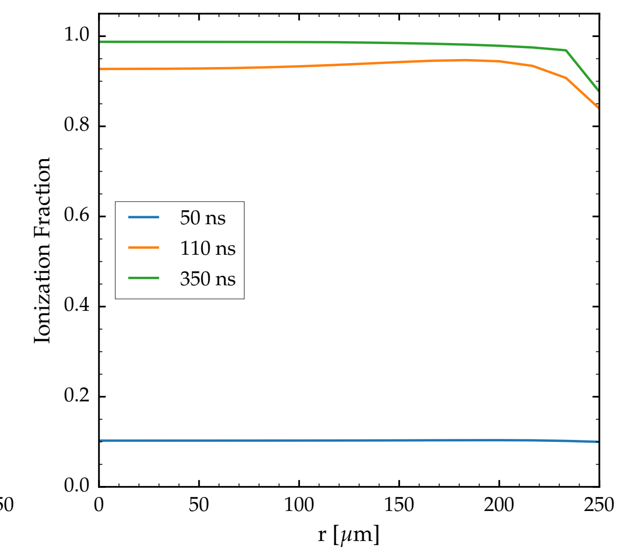
Capillary Benchmark Simulations in R-Z

- Phase I: Uniform Ohmic heating
  - *Rising, linear magnetic field profile*
- Phase II: Conductive cooling at wall
  - *Nearly total ionization of gas*
- Phase III: Steady state channeling
  - *Cooling at channel wall balances Ohmic heating along central axis*
  - *Parabolic channel formation due to thermal redistribution*



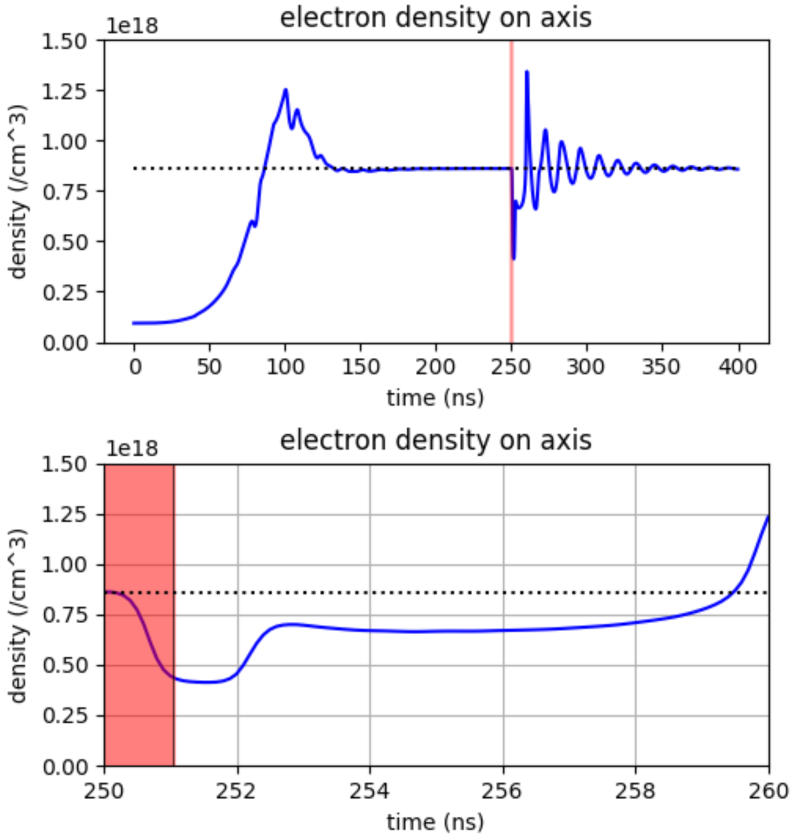


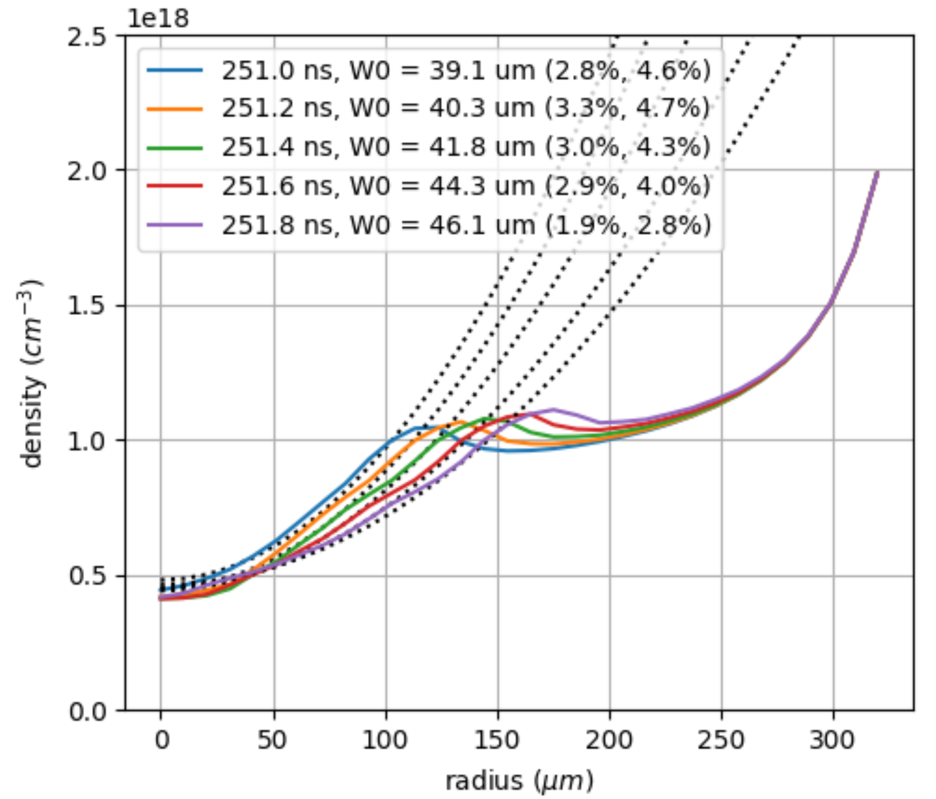




Modeling sub-channel formation via laser "heater"

- Proof of principle studies of laser deposition in pre-formed channel
  - *Gaussian laser, $\lambda_R >> L_Z$ produces collisional heating*
- For large pulse energies (~1 J), significant channeling observed, even at large background densities
  - *$\rho = 8 \times 10^{17}$ cm^{-3} → $\rho = 4 \times 10^{17}$ cm^{-3}, reduction of spot size from 75 to <50 micron*
  - *Density reduction scales laser intensity*





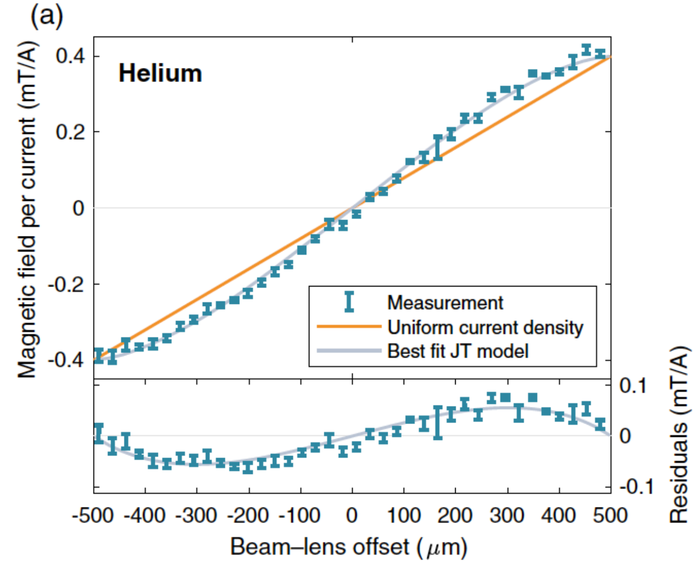
Capturing Nonlinear Current Distributions

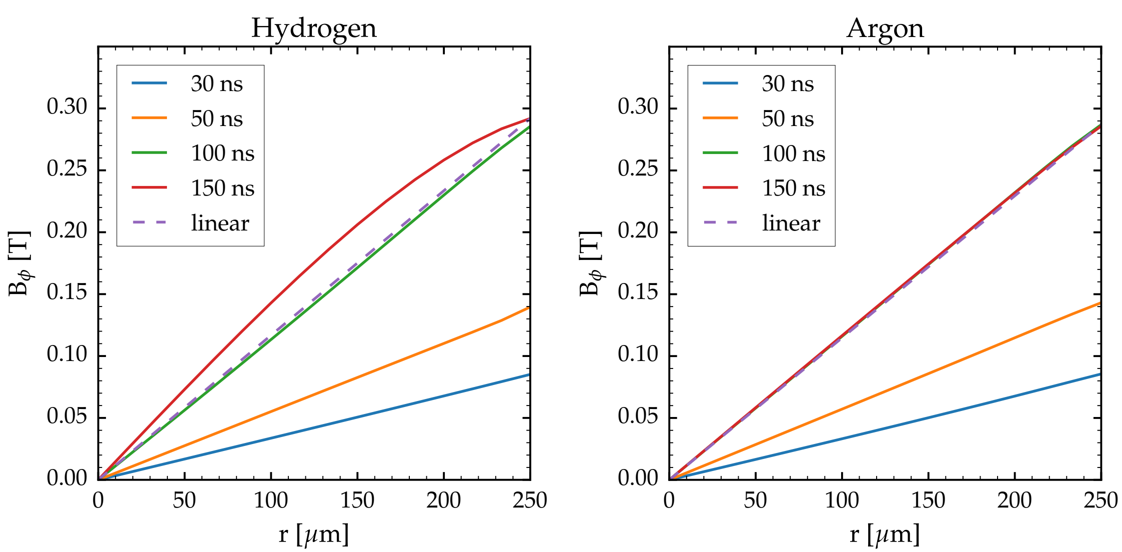
- Experimentally observed nonlinearities in field reproduced by simulations
  - *Temperature deviation drives current deviation**

$$J(r) \propto T_e(r)^{3/2}$$

*PRAB 20, 032803 (2017)

  - *Timescale of deviation from linearity is a function of mass*
    - ex. Argon maintains linear profile after 150 ns, whereas Hydrogen evolves





Phys. Rev. Lett. 121, 194801 (2018)

Optical plasma shaping for LPA targets

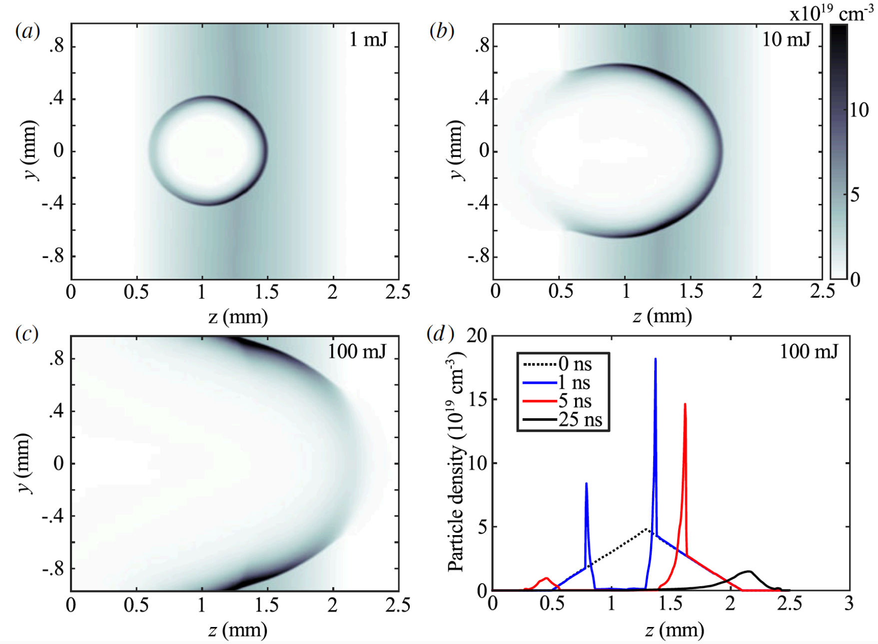
Laser deposition with pre-pulse for flexible target shaping

- Symmetric, robust, reproducible density profile

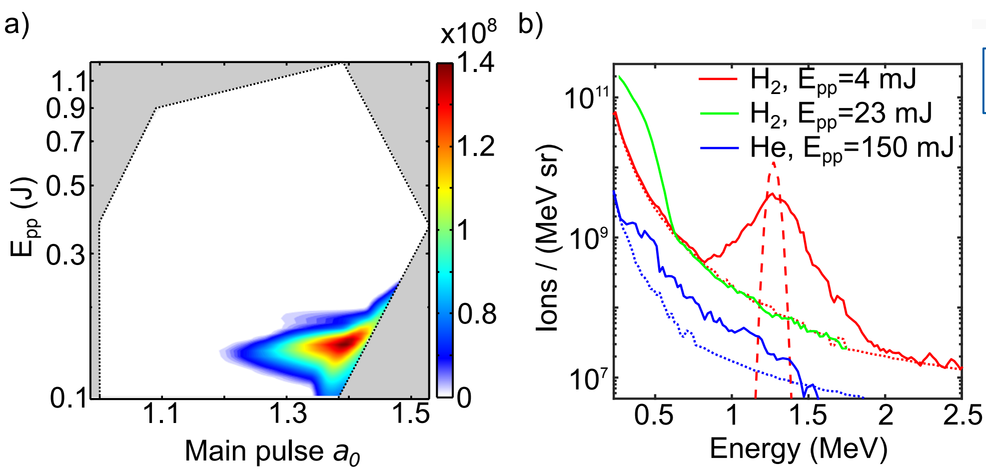
$$\frac{n}{n_0} = \frac{\gamma + 1}{\gamma - 1} \qquad \gamma \approx 1.3 - 1.4$$

- Controllable via pulse energy, timing, focal positon

Hydrodynamic modeling guides choice of parameters!



N.P. Dover et al., *J. Plasma Phys.*, **82**, 415820101 (2016).



O. Tresca et al., *PRL.*, **115**, 094802, (2015).

Applications for electron and ion acceleration schemes

- *Ions: Localize energy deposition*
- *Electrons: Localize injection*

Complementary to existing schemes (knife edge , gas jet, dual reservoir)

Summary of MHD applications

Modern plasma technologies can benefit from MHD modeling

1. Aberration free active plasma lenses for beam transport
   - *Coupling of low-emittance LWFA beams to diagnostics, or for staging*
   - *Choice of gas, discharge current, determine field strength and uniformity*
2. Plasma channel formation for laser guiding
   - *Parabolic channel formation for a range of central densities*
   - *Laser "heater" for sub-channel formation enables small matched spot*
3. Optical shaping of gas jets for laser plasma interactions
   - *Generation of narrow density spike through controlled pre-pulse*
   - *Viable for over-dense interactions as well as localized injection schemes*

We are actively developing MHD tools using the open-source FLASH code to support design and simulation of capillary systems

- *Continuing benchmark studies of capillary systems*
- *Cloud-based UI for FLASH is in development*

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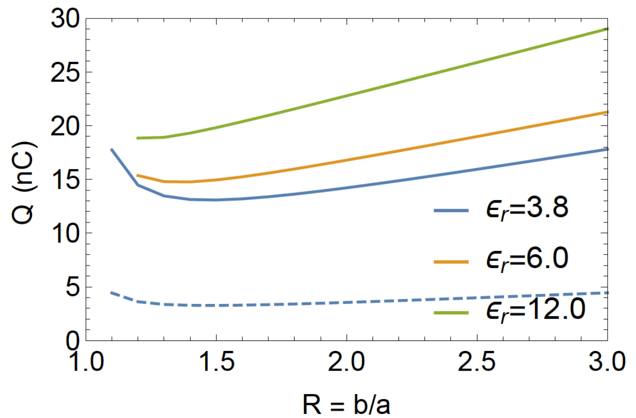
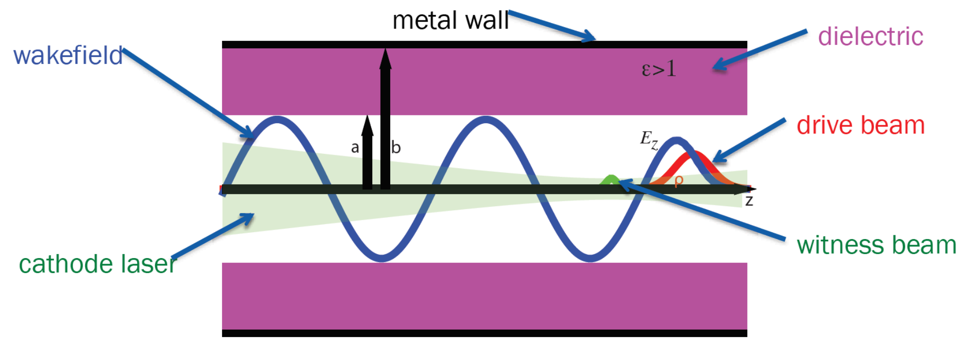
Modeling Dielectric and Hybrid Wakefield Accelerators

Structure-based acceleration for hybrid accelerator schemes

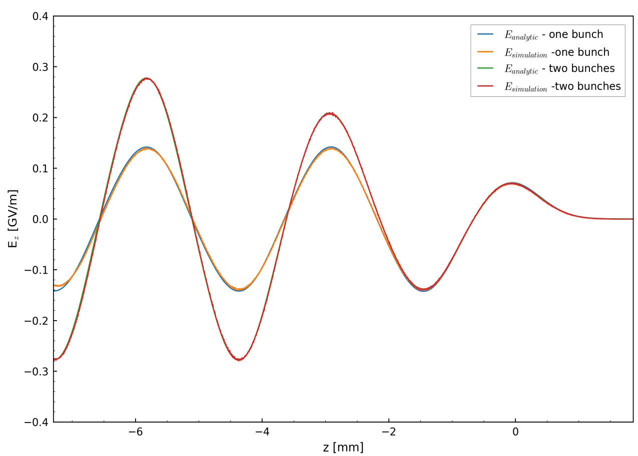
- Relaxed synchronization and trapping requirements

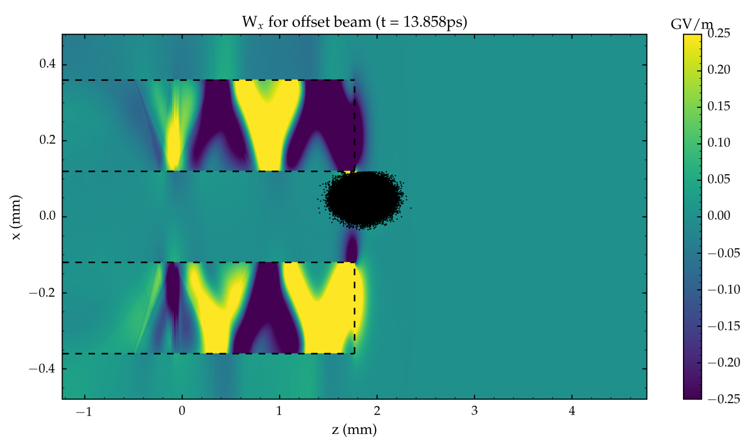




Courtesy F. Oshea

PIC simulations are well suited to capture physics of such systems





Large scale-length disparities between beam and structure are challenging

Modeling Novel Ionization Schemes

SSTF technique for plasma photocathode

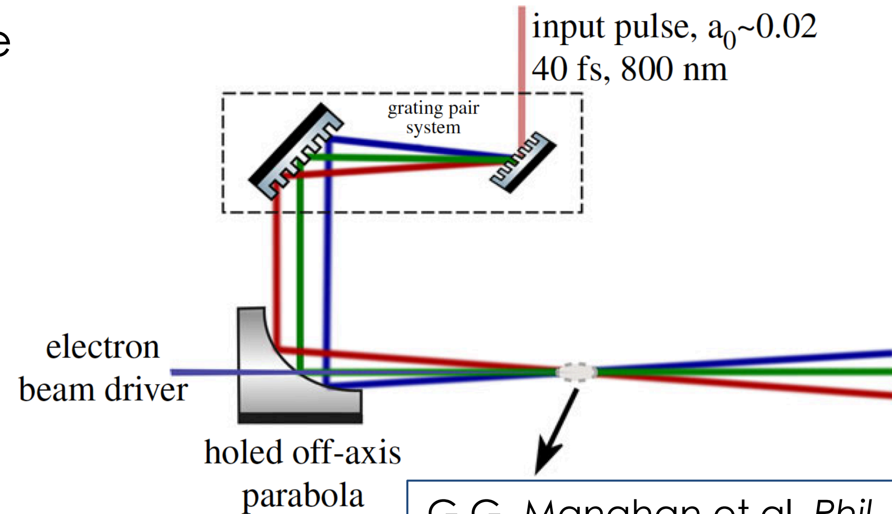
- Spatial and temporal chirp enable narrow region of peak intensity
- Superposition of Gaussian beamlets, spatially separated according to central frequency

Simulation is challenging

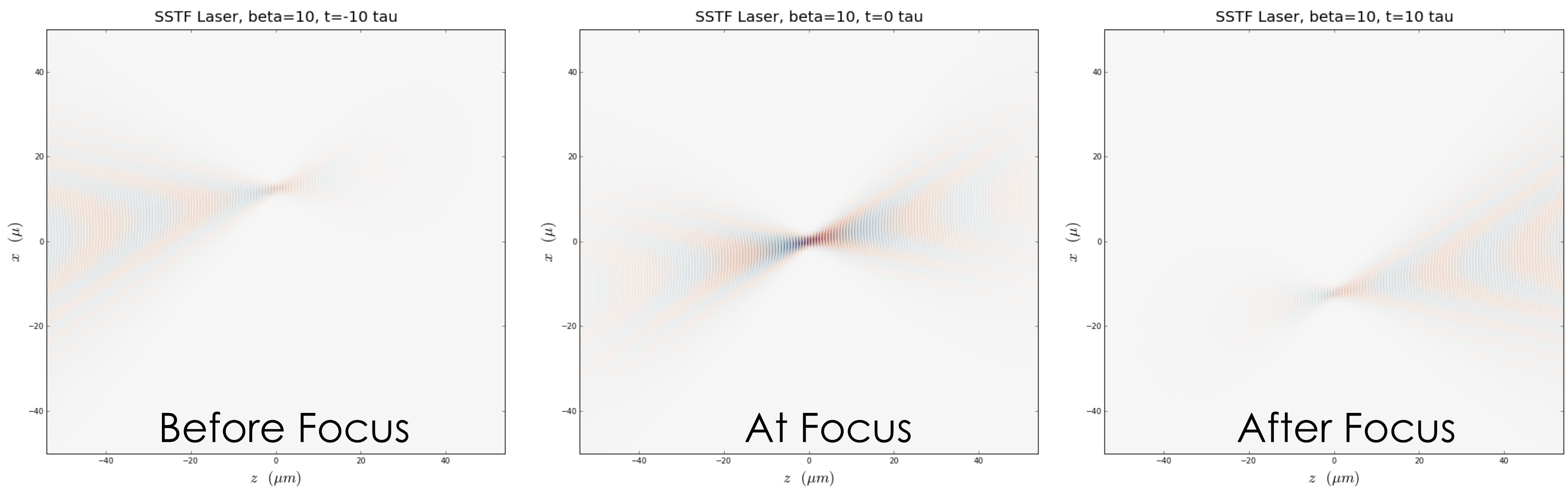
- Multiple antennae, small resolution, good numerical dispersion are required

Resort to analytical propagation

- Fast, high resolution, but not self-consistent



G.G. Manahan et al. *Phil. Trans. A.* **377** (2019)

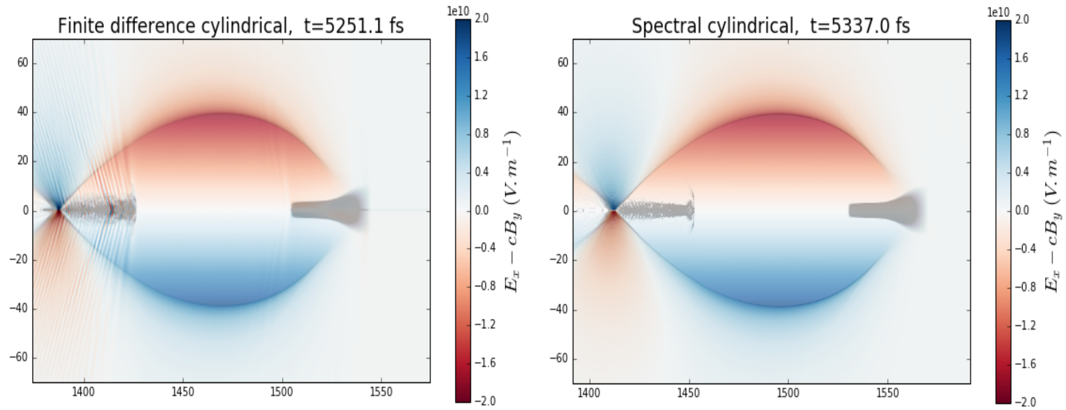


FBPIC - A Fourier-Bessel PSATD PIC Code

PSATD Algorithm presents unique advantages

- Sources deposited in Cartesian, gridded real space
- Apply Hankel transform to a Fourier-Bessel eigenmode basis
- Eigenmodes are analytically advanced
  - *No numerical Cherenkov*
  - *No numerical dispersion*
- For more details:

Comp. Phys. Comm. **203**, 66–82, 0010-4655 (2016).



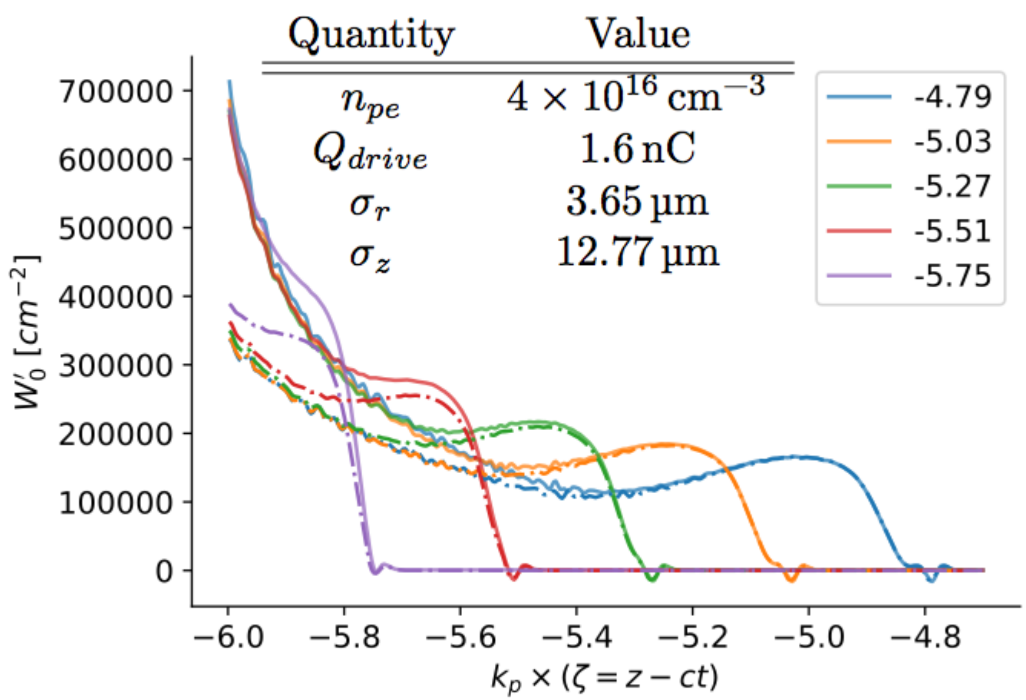
FBPIC Implementation permits fast prototyping

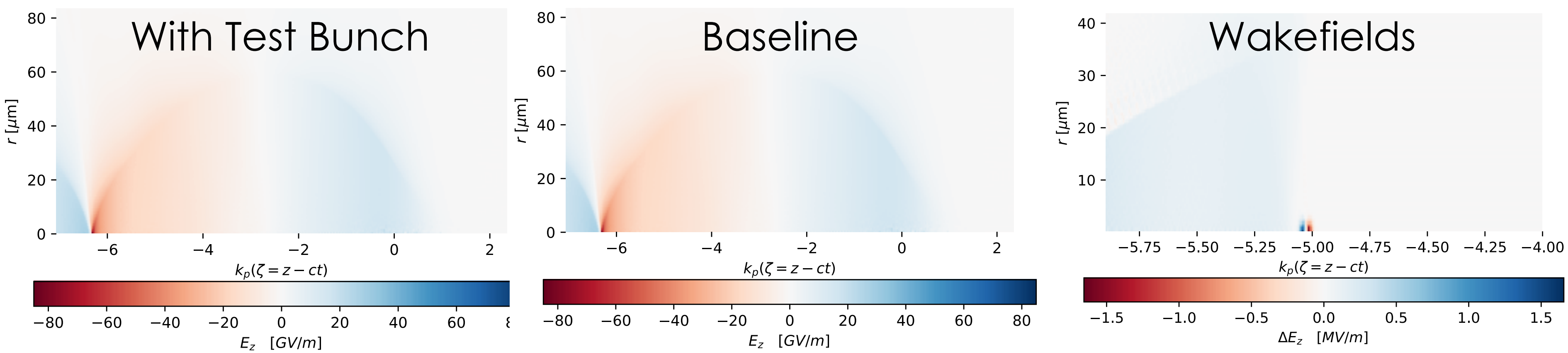
- Python interface accelerated using Numba JIT compiler
- GPU implementation of all major features
- Open source, available at: https://github.com/fbpic/fbpic
- Also available at https://jupyter.radiasoft.org

Calculation of Wake Functions from Loaded PWFA

Calculation of m = 0 wake from FBPIC simulation

- Perform baseline simulation with driver + witness bunch
- Introduce short, low-charge test bunch
- The difference in fields is a product of the wake functions





Promising PIC applications for ATF

- Modeling structure-based acceleration is resource intensive
  - Length-scale disparity between structure and beam is a boon for experiment, but a blight for simulations
  - Emphasize the adoption of novel techniques/architectures for speed
    - Spectral solvers, Lorentz boosted frame, mesh refinement
  - Conformal geometries may require development

- New ionization and injection schemes may require novel simulation tools
  - Analytical laser propagation coupled to plasma
  - Low density operation improves fidelity of this approach

- Spectral or pseudo-spectral algorithms improve LPA fidelity
  - Fast, low noise, free of numerical artifacts
    - Ideal for long timescale simulations
  - Compute subtle witness beam effects

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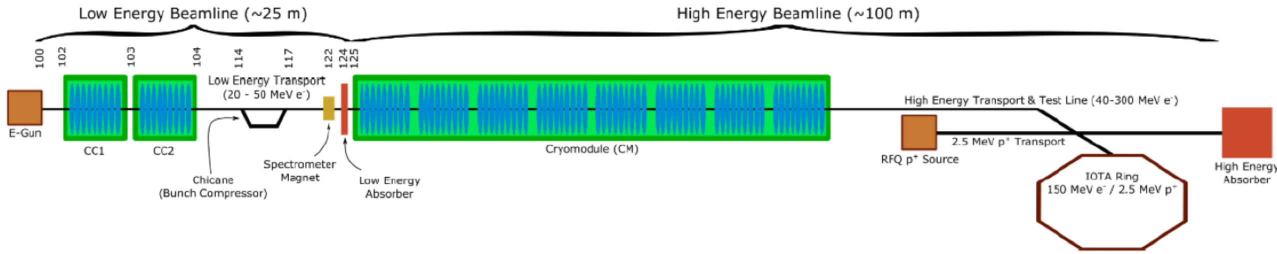
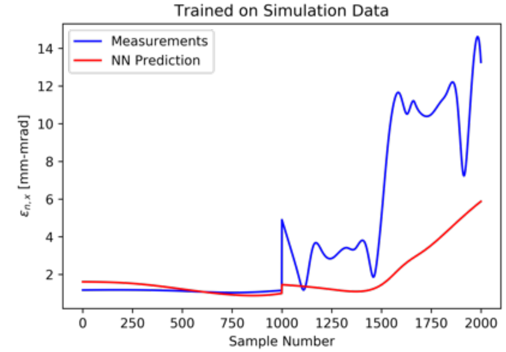
Virtual Diagnostics for electron beam tomography

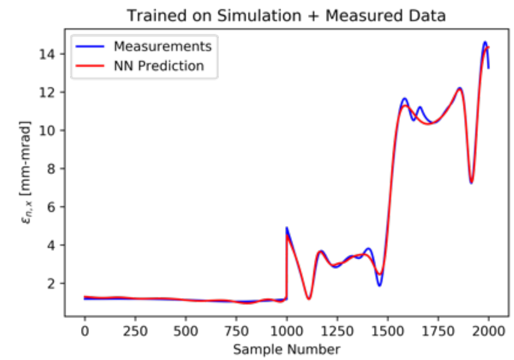


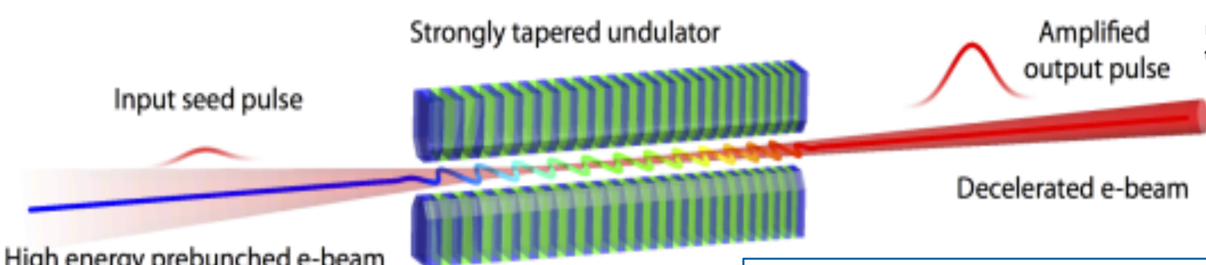


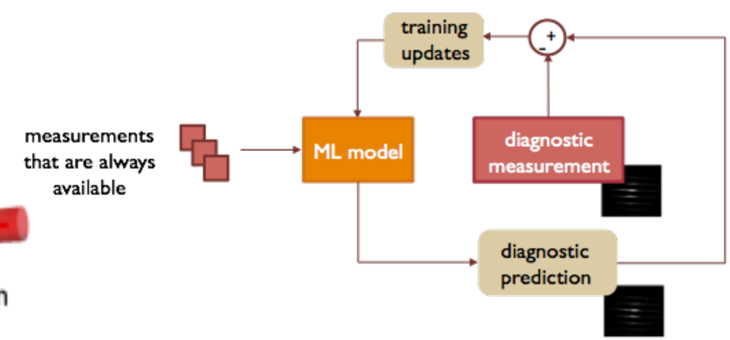
Virtual diagnostics emulate challenging and destructive measurements

- *Simulation provides the bulk of training set*
- *Leverage a small number of measurements to obtain good agreement*

- Example 1: Predict emittance from FAST photoinjector
  - *Sample solenoid strength and gun phase*
  - *Determine downstream σ_{ij} from upstream conditions*
- Example 2: Evaluate longitudinal phase space from LEA beamline
  - *Performance of TESSA undulator is sensitive to subtle variations resulting from CSR, wake fields, and longitudinal space charge*
  - *Couple simulations and intercepting diagnostics to train model for use during TESSA operation*



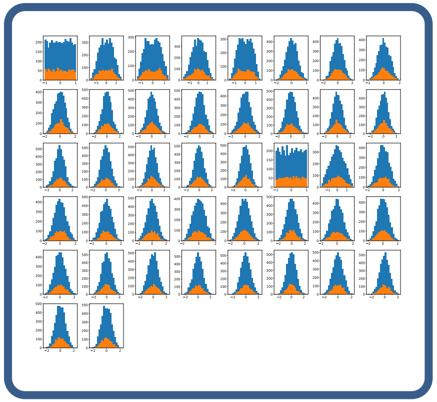




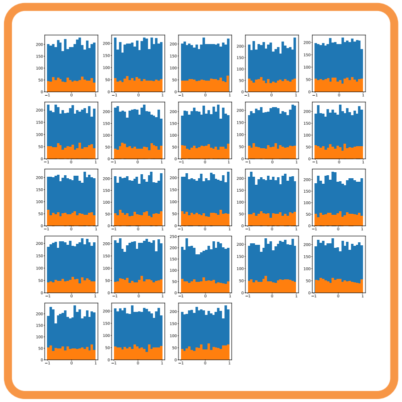
Duris et al., *New J. Phys.* **17**, 063036 (2015).

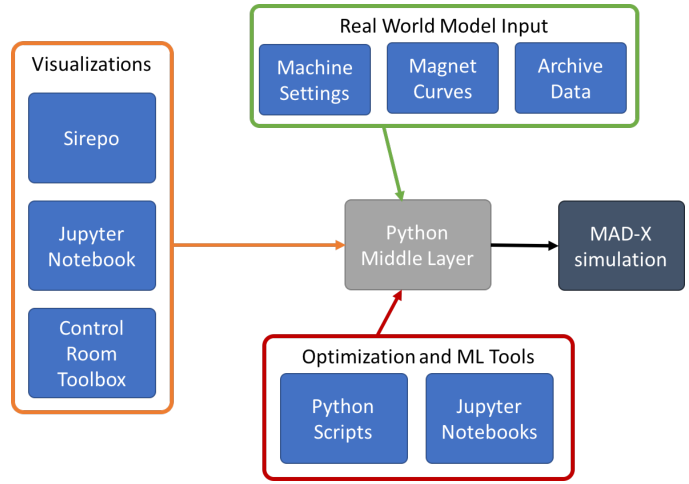
Beam steering in the BNL ATR with Machine Learning

Neural-Network Inputs
(BPMs and Initial Offsets)

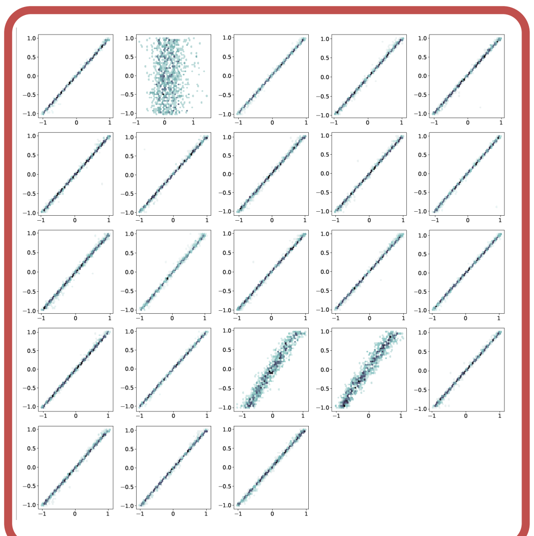


Neural-Network Outputs
(corrector settings)

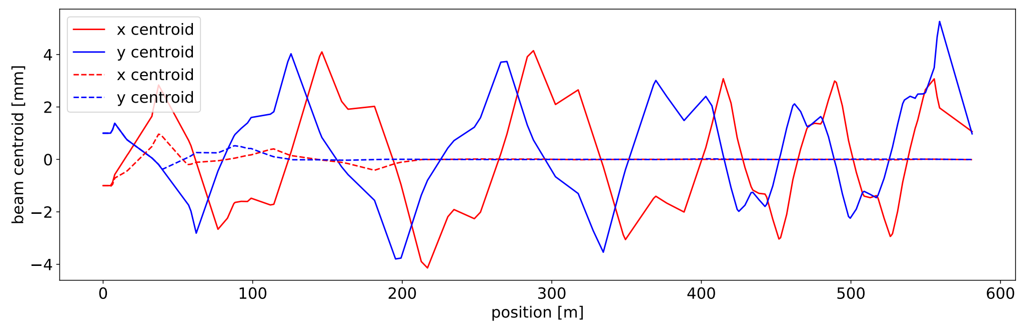




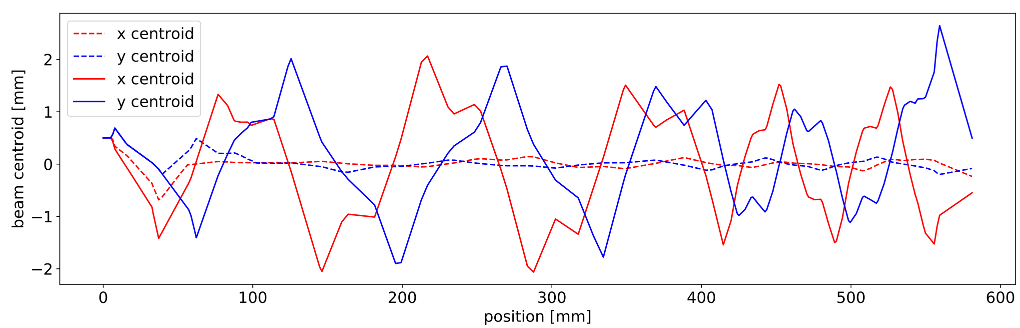
Neural-Network Performance
on the Validation set



Top: Initial beam trajectory and final beam trajectory using Nelder-Mead optimization on 23 correctors (2500 steps)

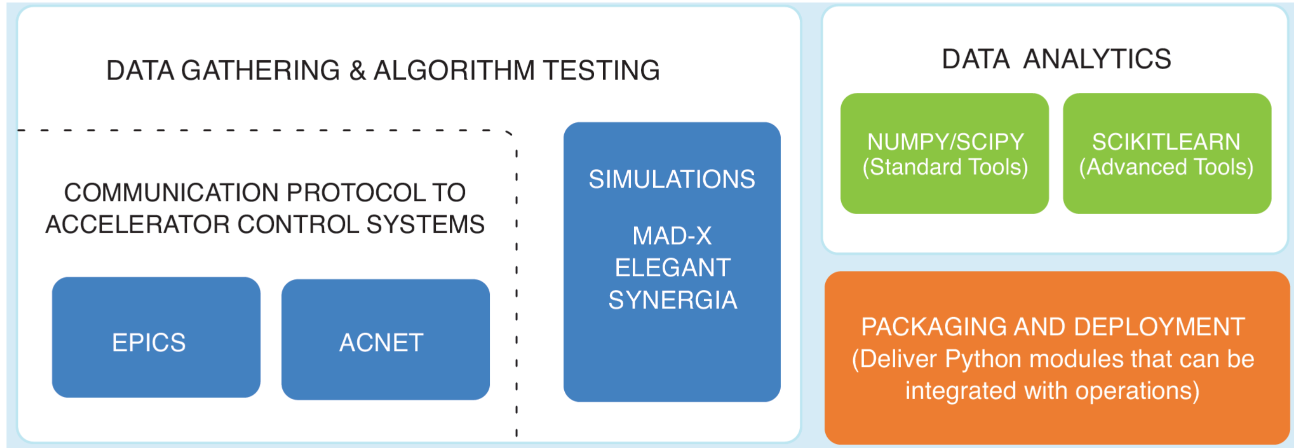


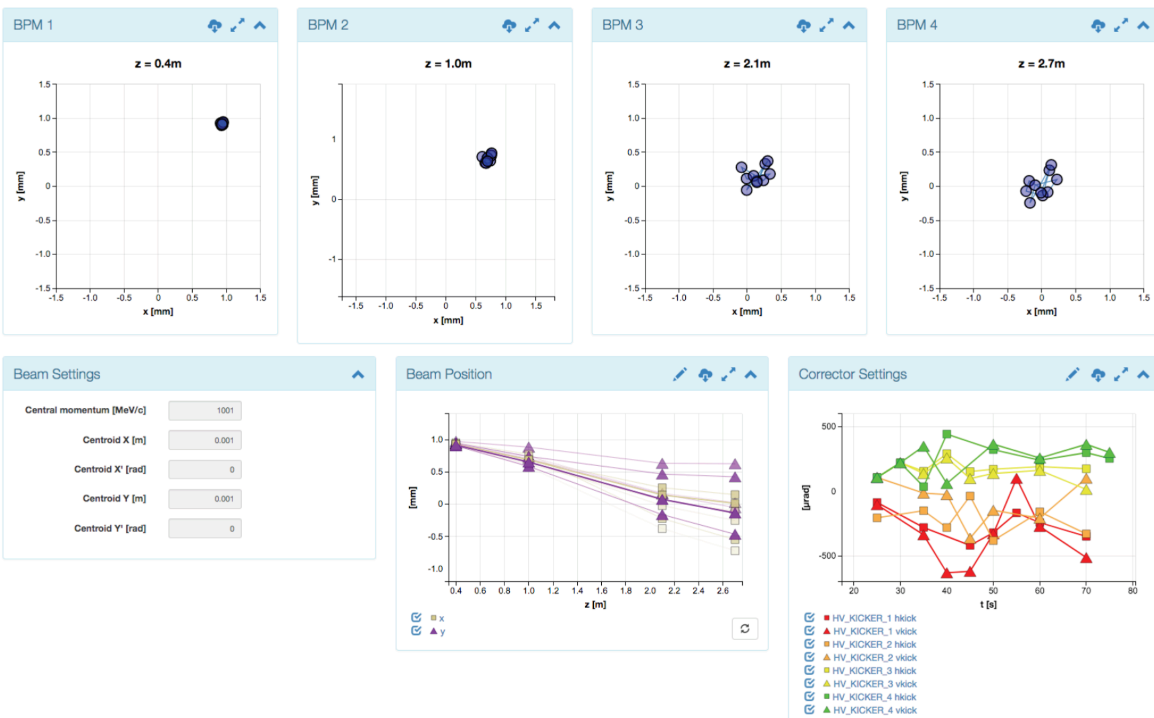
Bottom: Initial and final beam trajectory using inverse model (1 step)



Web-based controls toolkit for accelerators

- Interface between machine controls, simulation, and analysis
- Deployed as a Python module for seamless workflow





- Display machine settings, beam position, and relevant history
- Toggle diagnostics an corrector settings
- Integration with machine learning, optimization

Opportunities for Machine Learning at ATF

- Beam (and laser) phase space reconstruction
  - Diagnose photocathode phase errors
  - Reduce TCAV duty cycle for streak measurements
  - Improve M^2 measurement procedure

- Beamline tuning for fast reconfiguration
  - Develop online models for tuning parameters
  - Adjust laser parameters in response to environment

- Augment diagnostics laser-accelerated particle beams
  - Virtual interferogram for plasma density diagnostics
    - Reduce demands on probe pulse repetition rate, synchronization
  - Plasma temperature diagnostics
    - Reconstruct laser absorption with non-intercepting diagnostics

Many of these codes are accessible through Sirepo

- Sirepo is a cloud-based platform for scientific computing

- Supported Codes include:
  - *Particle Tracking: elegant, Synergia, Zgoubi,*
  - *Radiation: SRW (Synchrotron Radiation Workshop)*
  - *Particle-in-cell: Warp (Vacuum Nanoelectronic Devices + Plasma-Based Accelerators)*
  - *Electron Cooling: JSPEC*

- Advantages:
  - *No installation required*
  - *Share you work with a simple link*
  - *Archive and save simulations online*
  - *Export files for command-line execution*

- Try it out at https://sirepo.com/